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memorandum

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SUBJECT: (U) Adjoint-Weighted Leakage Time in SENSMG

I. Introduction

It is desired to compute the adjoint weighted leakage time τ_l for an α -eigenvalue problem.¹ The reciprocal of the leakage time is

$$\frac{1}{\tau_l} = \frac{\langle \psi^*, \mathbf{\Omega} \cdot \nabla \psi \rangle}{\langle \psi^*, \frac{1}{v} \psi \rangle}, \quad (1)$$

where ψ^* and ψ are the adjoint and forward α -eigenfunctions, respectively; v is neutron speed; and the angle brackets indicate an inner product over all independent variables, in this case space, energy, and angle.

This memo discusses the implementation of Eq. (1) in the multigroup neutron sensitivity code SENSMG (Refs. 2 and 3), which relies for the neutron transport on the multigroup discrete ordinates code PARTISN (Ref. 4).

It should be noted that a thorough discussion of various weighted and unweighted lifetimes and lifespans has been presented by Spriggs et al.^{5,6}

Section II of this report derives an equivalent expression for $1/\tau_l$ of Eq. (1) that is coded into SENSMG. Section III discusses calculating $1/\tau_l$ using a moments expansion of the streaming term in the numerator of Eq. (1). Section IV discusses angular fluxes and flux moments in inner products, and Sec. V presents results of a test problem. Section VI is a summary and discusses potential future work. The SENSMG input file for the test problem is listed in the appendix.

II. A Simple Equation for the Leakage Time

Start with the Boltzmann transport equation for the static eigenvalue α and α -eigenfunction ψ :

$$\begin{aligned} \mathbf{\Omega} \cdot \nabla \psi^g(\mathbf{r}, \mathbf{\Omega}) + \left(\Sigma_t^g(\mathbf{r}) + \frac{\alpha}{v^g} \right) \psi^g(\mathbf{r}, \mathbf{\Omega}) &= \sum_{g'=1}^G \int_{4\pi} d\mathbf{\Omega}' \Sigma_s^{g' \rightarrow g}(\mathbf{r}, \mathbf{\Omega}' \rightarrow \mathbf{\Omega}) \psi^{g'}(\mathbf{r}, \mathbf{\Omega}') \\ &+ \sum_{g'=1}^G \int_{4\pi} d\mathbf{\Omega}' \chi^{g' \rightarrow g} v \Sigma_f^{g'}(\mathbf{r}) \psi^{g'}(\mathbf{r}, \mathbf{\Omega}'). \end{aligned} \quad (2)$$

The notation is standard. Multiply both sides by the adjoint α -eigenfunction ψ^* , then integrate over angle and volume and sum over groups:

$$\begin{aligned} \sum_{g=1}^G \int dV \int_{4\pi} d\mathbf{\Omega} \psi^{*g}(\mathbf{r}, \mathbf{\Omega}) \mathbf{\Omega} \cdot \nabla \psi^g(\mathbf{r}, \mathbf{\Omega}) &+ \sum_{g=1}^G \int dV \int_{4\pi} d\mathbf{\Omega} \psi^{*g}(\mathbf{r}, \mathbf{\Omega}) \left(\Sigma_t^g(\mathbf{r}) + \frac{\alpha}{v^g} \right) \psi^g(\mathbf{r}, \mathbf{\Omega}) \\ &= \sum_{g=1}^G \int dV \int_{4\pi} d\mathbf{\Omega} \psi^{*g}(\mathbf{r}, \mathbf{\Omega}) \sum_{g'=1}^G \int_{4\pi} d\mathbf{\Omega}' \Sigma_s^{g' \rightarrow g}(\mathbf{r}, \mathbf{\Omega}' \rightarrow \mathbf{\Omega}) \psi^{g'}(\mathbf{r}, \mathbf{\Omega}') \\ &+ \sum_{g=1}^G \int dV \int_{4\pi} d\mathbf{\Omega} \psi^{*g}(\mathbf{r}, \mathbf{\Omega}) \sum_{g'=1}^G \int_{4\pi} d\mathbf{\Omega}' \chi^{g' \rightarrow g} v \Sigma_f^{g'}(\mathbf{r}) \psi^{g'}(\mathbf{r}, \mathbf{\Omega}'). \end{aligned} \quad (3)$$

Rearrange Eq. (3):

$$\begin{aligned} &\sum_{g=1}^G \int dV \int_{4\pi} d\mathbf{\Omega} \psi^{*g}(\mathbf{r}, \mathbf{\Omega}) \mathbf{\Omega} \cdot \nabla \psi^g(\mathbf{r}, \mathbf{\Omega}) \\ &= -\alpha \sum_{g=1}^G \int dV \int_{4\pi} d\mathbf{\Omega} \psi^{*g}(\mathbf{r}, \mathbf{\Omega}) \frac{1}{v^g} \psi^g(\mathbf{r}, \mathbf{\Omega}) - \sum_{g=1}^G \int dV \int_{4\pi} d\mathbf{\Omega} \psi^{*g}(\mathbf{r}, \mathbf{\Omega}) \Sigma_t^g(\mathbf{r}) \psi^g(\mathbf{r}, \mathbf{\Omega}) \\ &+ \sum_{g=1}^G \int dV \int_{4\pi} d\mathbf{\Omega} \psi^{*g}(\mathbf{r}, \mathbf{\Omega}) \sum_{g'=1}^G \int_{4\pi} d\mathbf{\Omega}' \Sigma_s^{g' \rightarrow g}(\mathbf{r}, \mathbf{\Omega}' \rightarrow \mathbf{\Omega}) \psi^{g'}(\mathbf{r}, \mathbf{\Omega}') \\ &+ \sum_{g=1}^G \int dV \int_{4\pi} d\mathbf{\Omega} \psi^{*g}(\mathbf{r}, \mathbf{\Omega}) \sum_{g'=1}^G \int_{4\pi} d\mathbf{\Omega}' \chi^{g' \rightarrow g} v \Sigma_f^{g'}(\mathbf{r}) \psi^{g'}(\mathbf{r}, \mathbf{\Omega}'). \end{aligned} \quad (4)$$

Divide by $\sum_{g=1}^G \int_{4\pi} d\Omega \psi^{*g}(\mathbf{r}, \Omega) \frac{1}{v^g} \psi^g(\mathbf{r}, \Omega)$:

$$\begin{aligned} & \frac{\sum_{g=1}^G \int dV \int_{4\pi} d\Omega \psi^{*g}(\mathbf{r}, \Omega) \Omega \cdot \nabla \psi^g(\mathbf{r}, \Omega)}{\sum_{g=1}^G \int dV \int_{4\pi} d\Omega \psi^{*g}(\mathbf{r}, \Omega) \frac{1}{v^g} \psi^g(\mathbf{r}, \Omega)} = -\alpha - \frac{\sum_{g=1}^G \int dV \int_{4\pi} d\Omega \psi^{*g}(\mathbf{r}, \Omega) \Sigma_t^g(\mathbf{r}) \psi^g(\mathbf{r}, \Omega)}{\sum_{g=1}^G \int dV \int_{4\pi} d\Omega \psi^{*g}(\mathbf{r}, \Omega) \frac{1}{v^g} \psi^g(\mathbf{r}, \Omega)} \\ & + \frac{\sum_{g=1}^G \int dV \int_{4\pi} d\Omega \psi^{*g}(\mathbf{r}, \Omega) \sum_{g'=1}^G \int_{4\pi} d\Omega' \Sigma_s^{g' \rightarrow g}(\mathbf{r}, \Omega' \rightarrow \Omega) \psi^{g'}(\mathbf{r}, \Omega')}{\sum_{g=1}^G \int dV \int_{4\pi} d\Omega \psi^{*g}(\mathbf{r}, \Omega) \frac{1}{v^g} \psi^g(\mathbf{r}, \Omega)} \\ & + \frac{\sum_{g=1}^G \int dV \int_{4\pi} d\Omega \psi^{*g}(\mathbf{r}, \Omega) \sum_{g'=1}^G \int_{4\pi} d\Omega' \chi^{g' \rightarrow g} v \Sigma_f^{g'}(\mathbf{r}) \psi^{g'}(\mathbf{r}, \Omega')}{\sum_{g=1}^G \int dV \int_{4\pi} d\Omega \psi^{*g}(\mathbf{r}, \Omega) \frac{1}{v^g} \psi^g(\mathbf{r}, \Omega)}. \end{aligned} \quad (5)$$

The left side of Eq. (5) is $1/\tau_l$ from Eq. (1). Rearrange the right side:

$$\begin{aligned} \frac{1}{\tau_l} = \alpha & \left[-1 + \left\{ - \frac{\sum_{g=1}^G \int dV \int_{4\pi} d\Omega \psi^{*g}(\mathbf{r}, \Omega) \Sigma_t^g(\mathbf{r}) \psi^g(\mathbf{r}, \Omega)}{\alpha \sum_{g=1}^G \int dV \int_{4\pi} d\Omega \psi^{*g}(\mathbf{r}, \Omega) \frac{1}{v^g} \psi^g(\mathbf{r}, \Omega)} \right. \right. \\ & + \frac{\sum_{g=1}^G \int dV \int_{4\pi} d\Omega \psi^{*g}(\mathbf{r}, \Omega) \sum_{g'=1}^G \int_{4\pi} d\Omega' \Sigma_s^{g' \rightarrow g}(\mathbf{r}, \Omega' \rightarrow \Omega) \psi^{g'}(\mathbf{r}, \Omega')}{\alpha \sum_{g=1}^G \int dV \int_{4\pi} d\Omega \psi^{*g}(\mathbf{r}, \Omega) \frac{1}{v^g} \psi^g(\mathbf{r}, \Omega)} \\ & \left. \left. + \frac{\sum_{g=1}^G \int dV \int_{4\pi} d\Omega \psi^{*g}(\mathbf{r}, \Omega) \sum_{g'=1}^G \int_{4\pi} d\Omega' \chi^{g' \rightarrow g} v \Sigma_f^{g'}(\mathbf{r}) \psi^{g'}(\mathbf{r}, \Omega')}{\alpha \sum_{g=1}^G \int dV \int_{4\pi} d\Omega \psi^{*g}(\mathbf{r}, \Omega) \frac{1}{v^g} \psi^g(\mathbf{r}, \Omega)} \right\} \right]. \end{aligned} \quad (6)$$

The term in curly braces in Eq. (6) is the sum of the relative first-order sensitivities of α to the density of each material in the system domain. The relative first-order sensitivity of α to the atom density N_i of material i is²

$$S_{\alpha, N_i} \equiv \frac{N_i}{\alpha} \frac{\partial \alpha}{\partial N_i} \quad (7)$$

(the relative first-order sensitivity of α to the mass density ρ_i of material i , S_{α, ρ_i} , is identical⁷ to S_{α, N_i}).

SENSMG already computed S_{α, N_i} for each material. The code now computes $1/\tau_l$ as simply

$$\frac{1}{\tau_l} = \alpha \left[-1 + \sum_{i=1}^I S_{\alpha, N_i} \right], \quad (8)$$

where I is the number of materials.

III. Moments of the Streaming Term

As noted in Ref. 1, the streaming term $\mathbf{\Omega} \cdot \nabla \psi$ can be written in terms of the scattering, fission, and removal terms. This is essentially what the derivation of Sec. II does. In this section, we do it explicitly.

Rearrange Eq. (2), replacing the angle integrals with sums over moments:

$$\begin{aligned} \mathbf{\Omega} \cdot \nabla \psi^g(\mathbf{r}, \mathbf{\Omega}) = & - \left(\frac{\alpha}{v^g} + \Sigma_t^g(\mathbf{r}) \right) \psi^g(\mathbf{r}, \mathbf{\Omega}) \\ & + \sum_{g'=1}^G \sum_{m=0}^M (2l_m + 1) \Sigma_{s, l_m}^{g' \rightarrow g}(\mathbf{r}) R_m(\mathbf{\Omega}) \phi_m^{g'}(\mathbf{r}) + \sum_{g'=1}^G \chi^{g' \rightarrow g} v \Sigma_f^{g'}(\mathbf{r}) \phi_0^{g'}(\mathbf{r}), \end{aligned} \quad (9)$$

where M is the number of moments associated with the scattering expansion order L and $R_m(\mathbf{\Omega})$ is the spherical harmonic function appropriate to the geometry.^{4,8} Multiply Eq. (9) by $R_m(\mathbf{\Omega})$ and integrate over angle for each m :

$$\begin{aligned} \int_{4\pi} d\mathbf{\Omega} R_m(\mathbf{\Omega}) \mathbf{\Omega} \cdot \nabla \psi^g(\mathbf{r}, \mathbf{\Omega}) = & - \left(\frac{\alpha}{v^g} + \Sigma_t^g(\mathbf{r}) \right) \int_{4\pi} d\mathbf{\Omega} R_m(\mathbf{\Omega}) \psi^g(\mathbf{r}, \mathbf{\Omega}) \\ & + \int_{4\pi} d\mathbf{\Omega} R_m(\mathbf{\Omega}) \sum_{g'=1}^G \sum_{m'=0}^M (2l_{m'} + 1) \Sigma_{s, l_{m'}}^{g' \rightarrow g}(\mathbf{r}) R_{m'}(\mathbf{\Omega}) \phi_{m'}^{g'}(\mathbf{r}) + \int_{4\pi} d\mathbf{\Omega} R_m(\mathbf{\Omega}) \sum_{g'=1}^G \chi^{g' \rightarrow g} v \Sigma_f^{g'}(\mathbf{r}) \phi_0^{g'}(\mathbf{r}), \end{aligned} \quad (10)$$

$m = 0, \dots, M.$

The first integral on the right side of Eq. (10) is the definition of the m th flux moment. Define an analogous moment of the streaming term:

$$\left[\mathbf{\Omega} \cdot \nabla \psi^g(\mathbf{r}, \mathbf{\Omega}) \right]_m \equiv \int_{4\pi} d\mathbf{\Omega} R_m(\mathbf{\Omega}) \mathbf{\Omega} \cdot \nabla \psi^g(\mathbf{r}, \mathbf{\Omega}). \quad (11)$$

In the scattering and fission terms, apply the orthogonality relation for spherical harmonics. It is complicated in general geometry given the associated Legendre polynomials, but the result is

$$\int_{4\pi} d\mathbf{\Omega} R_m(\mathbf{\Omega}) R_{m'}(\mathbf{\Omega}) = \frac{1}{2l_{m'} + 1} \delta_{mm'}. \quad (12)$$

Using Eqs. (11) and (12) in Eq. (10) yields an equation for each moment of the streaming term:

$$\left[\mathbf{\Omega} \cdot \nabla \psi^g(\mathbf{r}, \mathbf{\Omega}) \right]_0 = - \left(\frac{\alpha}{v^g} + \Sigma_t^g(\mathbf{r}) \right) \phi_0^g(\mathbf{r}) + \sum_{g'=1}^G \Sigma_{s, 0}^{g' \rightarrow g}(\mathbf{r}) \phi_0^{g'}(\mathbf{r}) + \sum_{g'=1}^G \chi^{g' \rightarrow g} v \Sigma_f^{g'}(\mathbf{r}) \phi_0^{g'}(\mathbf{r}), \quad (13)$$

$$\left[\mathbf{\Omega} \cdot \nabla \psi^g(\mathbf{r}, \mathbf{\Omega}) \right]_m = - \left(\frac{\alpha}{v^g} + \Sigma_t^g(\mathbf{r}) \right) \phi_m^g(\mathbf{r}) + \sum_{g'=1}^G \Sigma_{s, l_m}^{g' \rightarrow g}(\mathbf{r}) \phi_m^{g'}(\mathbf{r}), \quad m > 0. \quad (14)$$

Equation (1) can be evaluated using

$$\frac{1}{\tau_l} = \frac{\sum_{g=1}^G \int dV \sum_{m=0}^M (2l_m + 1) \phi_{IP,m}^{*g}(\mathbf{r}) [\mathbf{\Omega} \cdot \nabla \psi^g(\mathbf{r}, \mathbf{\Omega})]_m}{\sum_{g=1}^G \int dV \int_{4\pi} d\mathbf{\Omega} \psi^{*g}(\mathbf{r}, \mathbf{\Omega}) \frac{1}{v^g} \psi^g(\mathbf{r}, \mathbf{\Omega})}, \quad (15)$$

where subscript *IP* indicates that the inner product adjoint moment must be used rather than the calculational moment.⁸

IV. Inner Products: Angular Fluxes or Moments?

In Eq. (6), there are two instances of an integral of the form $\int_{4\pi} d\mathbf{\Omega} \psi^{*g}(\mathbf{r}, \mathbf{\Omega}) \psi^g(\mathbf{r}, \mathbf{\Omega})$. One is in the total cross section term and the other is in the $1/v$ term in the denominator, which also appears in Eq. (15). The most accurate way to compute this integral is to use a quadrature with angular fluxes:

$$\int_{4\pi} d\mathbf{\Omega} \psi^{*g}(\mathbf{r}, \mathbf{\Omega}) \psi^g(\mathbf{r}, \mathbf{\Omega}) \approx \sum_{n=1}^N w_n \psi_{-n}^{*g}(\mathbf{r}) \psi_n^g(\mathbf{r}), \quad (16)$$

where there are N ordinates, w_n is the weight associated with ordinate n , and $-n$ indicates the adjoint direction. Another way is to use an expansion of flux moments:

$$\int_{4\pi} d\mathbf{\Omega} \psi^{*g}(\mathbf{r}, \mathbf{\Omega}) \psi^g(\mathbf{r}, \mathbf{\Omega}) \approx \sum_{m=1}^M (2l_m + 1) \phi_{IP,m}^{*g}(\mathbf{r}) \phi_m^g(\mathbf{r}). \quad (17)$$

When using PARTISN for one-dimensional calculations, all of the angular fluxes are available. Thus, Eq. (16) should be used. For calculations in multiple dimensions, only the flux moments are available for volume integrals, so Eq. (17) has to be used.

In evaluating Eq. (8) [equivalent to Eq. (6)], SENSMSG uses angular fluxes for one-dimensional spheres and slabs and flux moments for two-dimensional cylinders.

V. Example

The example problem used the one-dimensional spherical homogeneous bare Jezebel critical benchmark.⁹ There is a homogenized-density version at a mass density of 15.61 g/cm³ and a realistic-density version at 15.82 g/cm³. They are both just critical. The realistic density of 15.82 g/cm³ was used with the larger radius of the 15.61-g/cm³ version, 6.39157 cm, in order to guarantee that there would be no problems with negative α -eigenvalues. The composition of the plutonium alloy is given in Table I. Its atom density was 4.083220672E-02 atoms/b·cm. The full SENSMSG input file is listed in the appendix.

Table I. Isotope Densities.

Isotope	Density (atoms/b·cm)
Pu-239	3.754542675E-02
Pu-240	1.774761157E-03
Pu-241	1.183143916E-04
Ga-69	8.472767111E-04
Ga-71	5.464277149E-04

An angular quadrature of S_{32} and fine mesh spacing of 0.005 cm were used. MENDF71X cross sections in 618 groups were used.

Values of $1/\tau_l$ computed using angular fluxes [Eq. (16)] in Eq. (8), flux moments [Eq. (17)] in Eq. (8), and flux moments [Eq. (17)] in Eq. (15) are compared for different scattering orders (i_{sct} in PARTISN) in Table II. The results show that Eq. (8) is equivalent to Eq. (15) when flux moments are used in both equations. The results also show a strong dependence of $1/\tau_l$ on the scattering order when flux moments are used, but not so much when angular fluxes are used. [It should be noted that PARTISN limits the number of expansion moments M in Eqs. (15) and (17) to be the same as the number of scattering moments associated with expansion order i_{sct} .] The results show that the difference between using angular fluxes and flux moments decreases to 0.02% at a scattering order of just 3.

Table II. $1/\tau_l$ (/sh).

Scattering Order	Angular Fluxes, Eq. (8)	Flux Moments, Eq. (8)	Flux Moments, Eq. (15)
0	2.963595E+00	1.773820E+00	1.773820E+00
1	3.028193E+00	3.174880E+00	3.174880E+00
3	3.026190E+00	3.026677E+00	3.026677E+00

The α -eigenvalue is listed for the different scattering orders in Table III. Interestingly, α 's dependence on scattering order is much greater than $1/\tau_l$'s on Table II.

Table III. α .

Scattering Order	α (/sh)
0	3.748596E-01
1	2.218024E-02
3	4.482678E-02

VI. Summary and Future Work

SENSMG now computes the reciprocal of the adjoint weighted leakage time τ_l for α -eigenvalue problems. Angular fluxes are used for inner products in one-dimensional slabs and spheres, and flux moments are used in two-dimensional cylinders. In some cases, including the problem presented in this memo, a flux moments expansion can be quite accurate. More study should be done to determine the accuracy limits of the approximation for this purpose.

Many other adjoint-weighted lifetimes^{5,6} can be computed using SENSMG.

The sensitivity of $1/\tau_l$ to arbitrary input parameter a_x may be of interest. From Eqs. (7) and (8),

$$\left(\frac{1}{\tau_l} \right) = -\alpha + \sum_{i=1}^l N_i \frac{\partial \alpha}{\partial N_i}. \quad (18)$$

Taking the derivative yields

$$\frac{\partial}{\partial a_x} \left(\frac{1}{\tau_l} \right) = -\frac{\partial \alpha}{\partial a_x} + \sum_{i=1}^I \frac{\partial N_i}{\partial a_x} \frac{\partial \alpha}{\partial N_i} + \sum_{i=1}^I N_i \frac{\partial^2 \alpha}{\partial a_x \partial N_i}. \quad (19)$$

We are presently working on second derivatives of responses in neutron transport problems. With some work, it would be possible to evaluate Eq. (19) exactly.

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APPENDIX A INPUT FILE

SENSMG INPUT FILE

```
Pu-239 Jezebel (benchmark radius, realistic density)
alpha sph
mendf71x      / libname
1              / no of materials
1 94239 -9.42090E-01 94240 -4.47189E-02 94241 -2.99354E-03 31069 -6.12984E-
03 31071 -4.06790E-03 / Pu-alloy
-15.82        / densities
1              / no of shells
6.39157       / outer radii
1              / material nos
0              / number of edit points
0              / number of reaction-rate ratios
```

The following command line was used to run the input file above:

```
${SENSMG} -i jezebel -isct ${isct} -ngroup 618 -np 1 -aflxfrm 0
```

where C-SHELL variable `${isct}` was 0, 1, or 3.